# Revealing Hidden Coherence in Partially Coherent Light

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Coherence and correlations represent two related properties of a compound system. The system can be, for instance, the polarization of a photon, which forms part of a polarization-entangled two-photon state, or the spatial shape of a coherent beam, where each spatial mode bears different polarizations. Whereas a local unitary transformation of the system does not affect its coherence, global unitary transformations modifying both the system and its surroundings can enhance its coherence, transforming mutual correlations into coherence. The question naturally arises of what is the best measure that quantifies the correlations that can be turned into coherence, and how much coherence can be extracted. We answer both questions, and illustrate its application for some typical simple systems, with the aim at illuminating the general concept of enhancing coherence by modifying correlations.

*Introduction.*—Coherence is one of the most important concepts needed to describe the characteristics of a stream of photons [1, 2], where it allows us to characterize the interference capability of interacting fields. However its use is far more general as it plays a striking role in a whole range of physical, chemical, and biological phenomena [3]. Measures of coherence can be implemented using classical and quantum ideas, which lead to the question of in which sense quantum coherence might deviate from classical coherence phenomena [4], and to the evaluation of measures of coherence [5–7].

Commonly used coherence measures consider a physical system as a whole, omitting its structure. The knowledge of *the internal distribution of coherence* between subsystems and their correlations becomes necessary for predicting the evolution (migration) of coherence in the studied system. The evolution of a twin beam from the near field into the far field represents a typical example occurring in nature [8]. The creation of entangled states by merging the initially separable incoherent and coherent states serves as another example [7]. Or, in quantum computing the controlled-NOT gate entangles (disentangles) two-qubit states [9, 10], at the expense (in favor) of coherence. Many quantum metrology and communication applications benefit from correlations of entangled photon pairs originating in spontaneous parametric down-conversion [11–13]. Even separable states of photon pairs, i.e. states with suppressed correlations, are very useful, e.g., in the heralded single photon sources [14, 15]. For all of these, and many others, examples the understanding of common evolution of coherence and correlations is crucial.

The Clauser-Horne-Shimony-Holt (CHSH) Bell's-like inequality [16–18] has been usually considered to quantify nonclassical correlations present between physically sepa-rated photons that are entangled and so they can violate the bound set by the inequality. However, correlations of a similar nature can also exist when considering different degrees of freedom of a single system [19, 20]. The CHSH inequality can also be violated when considering intrabeam correlations between different degrees of freedom of intense beams, coherent or not [21]. This, sometimes referred to as *nonquantum entanglement*, or inseparability of degrees of freedom, has been considered [22, 23] as a tool to shed new light into certain characteristics of classical fields, by applying techniques usually restricted to a quantum scenario.

When the violation of the CHSH inequality between subsystems and the degree of first-order coherence, which characterizes the internal coherence of a physical subsystem [1], are combined together, it is possible to define a measure that encompasses all coherences and correlations in the system. This measure has been experimentally examined by Kagalwala *et al.* [24]. One fundamental problem of their formulation is that it varies under global unitary transformations. This means that, from this point of view, the amount of coherence in the system can be changed.

This behavior has several general consequences for any partially coherent (mixed) state. First, the main point is that the coherence of each subsystem can be increased by means of a suitable unitary transformation affecting the whole system. So the *hidden coherence* stored in the correlations between two subsystems is made available. Second, for pure states, the roles of the degree of entanglement between subsystems, quantified by the concurrence [25, 26], and the maximum violation of the CHSH inequality ($B_{max}$) [18] are interchangeable. However, this is not true for mixed states, where the maximal violation can take place for states that are not maximally entangled [27]. This raises the question of what is the appropriate measure to

quantify *hidden coherence* unveiled by global unitary transformations: the degree of entanglement (concurrence) or $B_{\max}$.

In this Letter, we solve these two puzzles. First, given a generally mixed state, or equivalently a partially coherent light beam, *we determine what is the maximum and minimum first-order coherence the subsystems can show under global unitary transformations.* This will reveal how much hidden coherence is present in the correlations between subsystems. Second, we will determine *if these maximal and minimal coherences are related to states with the maximal (minimal) degree of entanglement, or maximal or minimal violation of the CHSH inequality.* This will solve the question of which of the two measures is the appropriate one to quantify hidden coherence. Our main results are expressed in two theorems valid for any mixed two-qubit quantum state, and their implication is illustrated by applying the theorems to four well-known classes of quantum states.

We restrict our attention to coherence manipulations by a general global unitary transformation. Experimentally, they can be implemented by various logical gates [13, 28, 29]. The coherence limits can be also viewed as *the maximal coherence* that a logical gate can provide for a given state, which is related to the entanglement power of a unitary operation [30].

*General considerations.*—Let us consider a $2 \times 2$ dimensional quantum state, $\hat{\rho}$, composed of subsystems $A$ and $B$. The state $\hat{\rho}$ can be generally written (spectral decomposition) as $\hat{\rho} = V \hat{E} V^{\dagger}$ [13], where $\hat{E}$ is a diagonal matrix with eigenvalues that satisfy $\sum_i \lambda_i = 1$ and $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$. The matrix $V$ contains the corresponding eigenvectors. Each subsystem is characterized by the corresponding density matrix, $\hat{\rho}_A$ and $\hat{\rho}_B$. The degree of first-order coherence of each subsystem is given $D_{A,B} = \sqrt{2\mathrm{Tr}[\hat{\rho}_{A,B}^2] - 1}$ [2]. We introduce here a measure of coherence for both subsystems when they are considered independently $D^2 = (D_A^2 + D_B^2)/2$. When both subsystems are coherent, one has $D = 1$, while only if both subsystems show no coherence, $D = 0$.

*Minimum first-order coherence.*—There exists a unitary transformation $U$ that when applied to $\hat{\rho}$ generates a new state $\hat{\rho}' = U\hat{\rho}U^{\dagger}$, so that the coherence $D$ vanishes and the violation of the CHSH is maximized with value [18, 31]

$$B_{\max} = 2\sqrt{2}\sqrt{(\lambda_1 - \lambda_4)^2 + (\lambda_2 - \lambda_3)^2}. \qquad (1)$$

The unitary transformation has the form $U = MV^{\dagger}$, where

$$M = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \end{pmatrix}. \qquad (2)$$

It is straightforward to show (see Supplemental Material) that after the transformation $MV^{\dagger}$, $D_A = D_B = 0$, there-

fore $D = D_{\min} = 0$. One can always achieve no coherence for both subsystems. Therefore, the state with minimal coherence is the state that provides maximal violation of the CHSH inequality and it corresponds to the so-called Bell diagonal state [31].

The degree of entanglement (concurrence) of Bell diagonal states is $C_{BD} = \max\{0, 2\lambda_1 - 1\}$ [31]. The maximum concurrence that can be achieved by a unitary operation applied on $\hat{\rho}$ is $C_{\max} = \max\{0, \lambda_1 - \lambda_3 - 2\sqrt{\lambda_2 \lambda_4}\}$ [32]. As we will see in example I, $C_{BD} \leq C_{\max}$ can happen for mixed states, which highlights the preference for using $B_{\max}$ over the concurrence for quantifying the coherence available for each subsystem.

*Maximum first-order coherence.*—There exists a unitary transformation $U$ that when applied to an arbitrary state $\hat{\rho}$ generates a new state $\hat{\rho}' = U\hat{\rho}U^{\dagger}$ that maximizes the coherence $D$ with value

$$D_{\max}^2 = (\lambda_1 - \lambda_4)^2 + (\lambda_2 - \lambda_3)^2 \qquad (3)$$

and yields a violation of CHSH that is minimal, with value

$$B_{\max} = 2|\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4|. \qquad (4)$$

The unitary transformation $U$ has the form $U = V^{\dagger}$.

The resulting state is a diagonal separable state, as it is shown in the Supplemental Material.

$D_{\max}$ can be called the *degree of available coherence*, since it represents the maximum first-order coherence that can be unveiled under a global unitary transformation. As we will show in example I below, correlations can be a source of coherence for a subsystem even when the CHSH inequality is not violated, i.e., $B_{\max} \leq 2$, and therefore the state is not entangled. Importantly, $D_{\max}$ is associated to a state with the minimum violation of the CHSH inequality, highlighting again the outstanding role of $B_{\max}$ over concurrence when considering the maximum and minimum values of the degree of coherence available.

We will now consider four examples where we apply the results mentioned above.

*Example I: Maximally nonlocal mixed state (MNMS).*—In a nonlinear process designed to generate entanglement in polarization [33, 34], the state generated at the output of the nonlinear crystal can be generally written in the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ as [27, 35]

$$\hat{\rho}_{\mathrm{MNMS}} = \begin{pmatrix} 1/2 & 0 & 0 & \epsilon/2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \epsilon/2 & 0 & 0 & 1/2 \end{pmatrix} \quad \text{where } \epsilon \in \langle 0, 1\rangle. \qquad (5)$$

The purity of the state is $P = \mathrm{Tr}[\hat{\rho}_{\mathrm{MNMS}}^2] = (1 + \epsilon^2)/2$. The spectral representation of this state writes $\hat{\rho}_{\mathrm{MNMS}} = 1/2\,(1 + \epsilon)|\Phi^+\rangle\langle\Phi^+| + 1/2\,(1 - \epsilon)|\Phi^-\rangle\langle\Phi^-|$ This state is a Bell diagonal state, so it produces a maximal violation of the CHSH inequality. For each value of $\epsilon$, the state $\hat{\rho}_{\mathrm{MNMS}}$
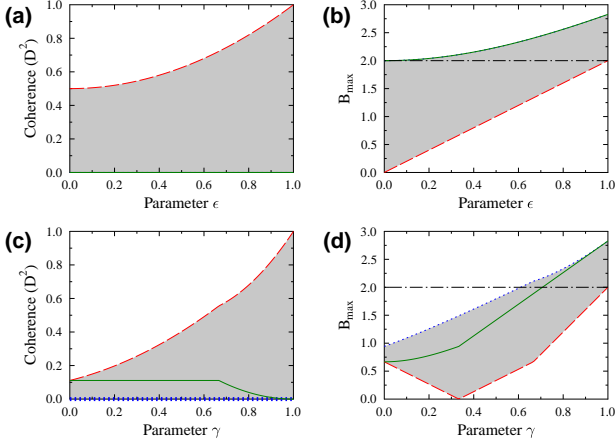
FIG. 1. Coherence ($D^2$) and maximal violation of the CHSH inequality ($B_{\max}$) for (a) and (b): example I ($\hat{\rho}_{\mathrm{MNMS}}$), and (c) and (d): example II ($\hat{\rho}_{\mathrm{MEMS}}$). Green lines depict the values of the original state, prior to any unitary transformation. The maximal coherence and minimal violation of the CHSH inequality are marked by dashed-red lines, and the minimal coherence and maximal violation of the CHSH inequality are marked by dotted-blue lines. The black dashed-dotted line represents the classical correlation limit $B_{\max} = 2$. Grey areas correspond to all admissible values achievable by all unitary operations.

can be transformed using unitary operations to a new state $\hat{\rho}'_{\mathrm{MNMS}}$ with new values of $D^2$ [see Fig. 1(a)] and $B_{\max}$ [see Fig. 1(b)]. The grey areas in the figures show all possible values of $D^2$ and $B_{\max}$. In all cases presented here, and shown in Figs. 1–2, we performed extensive numerical simulations [36] generating $10^6$ randomly generated unitary operations for each value of parameters, to check all of our predictions.

All of these values lie in intervals limited by states with minimal and maximal coherence. The state already yields minimal coherence ($D_A = D_B = 0$) and maximal violation of the CHSH inequality, as given by Eq. (1) [dotted-blue lines in Figs. 1(a) and 1(b)]

$$D_A = D_B = 0, \qquad B_{\max} = 2\sqrt{1 + \epsilon^2}. \qquad (6)$$

The case of maximal coherence and minimal violation of the CHSH inequality is given by Eqs. (3) and (4) [dashed-red lines in Figs. 1(a) and 1(b)]

$$D^2_{\max} = \frac{1 + \epsilon^2}{2}, \qquad B_{\max} = 2|\epsilon|. \qquad (7)$$

The degree of entanglement of the quantum state with minimum first-order coherence ($D_A = D_B = 0$), which corresponds to the maximal violation of the CHSH inequality, is $C_{BD} = \epsilon$. However, the maximum entanglement that can be achieved with a unitary operation is $C_{\max} = (1 + \epsilon)/2$. Therefore $C_{BD} < C_{\max}$. This shows the relevant role $B_{\max}$

over the concurrence. The state which achieves minimal first-order coherence for a subsystem is also the state that maximally violates the CHSH inequality, but not the state that achieves maximum entanglement.

*Example II: Maximally entangled mixed state (MEMS)*— This state is defined as [37, 38]

$$\hat{\rho}_{MEMS} = \begin{cases} \begin{pmatrix} 1/3 & 0 & 0 & \gamma/2 \\ 0 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \gamma/2 & 0 & 0 & 1/3 \end{pmatrix} & \text{for } 0 \leq \gamma \leq \frac{2}{3} \\[20pt] \begin{pmatrix} \gamma/2 & 0 & 0 & \gamma/2 \\ 0 & 1-\gamma & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \gamma/2 & 0 & 0 & \gamma/2 \end{pmatrix} & \text{for } \frac{2}{3} \leq \gamma \leq 1 \end{cases}$$
$$(8)$$

It maximizes the value of the concurrence for a given value of the purity. We have chosen the phases to be zero for the sake of simplicity. The purity is equal to $P = \frac{1}{3} + \frac{\gamma^2}{2}$ for $0 \leq \gamma \leq \frac{2}{3}$ and $P = \gamma^2 + (1 - \gamma)^2$ for $\frac{2}{3} \leq \gamma \leq 1$. When the state is transformed to the new state using unitary operations [see Figs. 1(c) and 1(d)], we find that for $0 \leq \gamma \leq \frac{2}{3}$ the minimal coherence and maximal violation of the CHSH are [dotted-blue lines in Figs. 1(c) and 1(d)]

$$D_A = D_B = 0, \qquad B_{\max} = 2\sqrt{2}\sqrt{\frac{\gamma^2}{4} + \left(\frac{1}{3} + \frac{\gamma}{2}\right)^2} \qquad (9)$$

and the maximal coherence and minimal violation of the CHSH are [dashed-red lines in Figs. 1(c) and 1(d)]

$$D^2_{\max} = \frac{\gamma^2}{4} + \left(\frac{1}{3} + \frac{\gamma}{2}\right)^2, \qquad B_{\max} = 2\left|\gamma - \frac{1}{3}\right|. \qquad (10)$$

For $\frac{2}{3} \leq \gamma \leq 1$, these limits are [dotted-blue and dashed-red lines in Figs. 1(c) and 1(d)]

$$D_A = D_B = 0, \qquad B_{\max} = 2\sqrt{2}\sqrt{\gamma^2 + (1 - \gamma)^2} \qquad (11)$$

and

$$D^2_{\max} = \gamma^2 + (1 - \gamma)^2, \qquad B_{\max} = 2|2\gamma - 1|. \qquad (12)$$

The green lines in Figs. 1(c) and 1(d) show the actual value of $D^2$ and $B_{\max}$, prior to the application of any unitary transformation.

*Example III: State considered in [24].*—Kagalwala *et al.* investigated (example C) a state whose density matrix writes

$$\hat{\rho}_{EXC}(p) = \frac{1}{2} \begin{pmatrix} 1-p & 0 & 1-p & 0 \\ 0 & p & ip & 0 \\ 1-p & -ip & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad \text{where } p \in \langle 0, 1 \rangle.$$
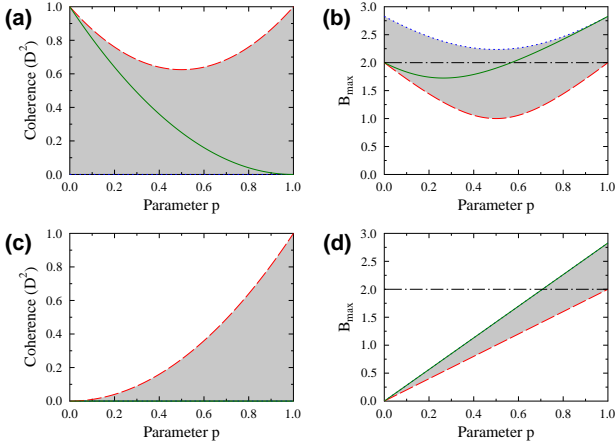$$(13)$$

FIG. 2. Coherence ($D^2$) and maximal violation of the CHSH inequality ($B_{\max}$) for (a) and (b): example III ($\hat{\rho}_{\mathrm{EXC}}$); and (c) and (d): example IV ($\hat{\rho}_W$). Green lines depict the values of the original state, prior to any unitary transformation. The maximal coherence and minimal violation of the CHSH inequality are marked by dashed-red lines, and the minimal coherence and maximal violation of the CHSH inequality are marked by dotted-blue lines. The black dashed-dotted line represents the classical correlation limit $B_{\max} = 2$. Grey areas correspond to all admissible values achievable by all unitary operations.

The purity of this state is $P = 1 - \frac{3}{2}p + \frac{3}{2}p^2$. In Figs. 2(a) and 2(b) all possible values of $D^2$ and $B_{\max}$ are shown for this particular case. The boundaries of the grey areas are formed by the states with minimal coherence and maximal violation of the CHSH inequality [39]

$$D_1 = D_2 = 0, \quad B_{\max} = 2\sqrt{2}\sqrt{1 - \frac{3}{2}p + \frac{3}{2}p^2} \quad (14)$$

and the maximal coherence and correspondingly minimal violation of the CHSH inequality

$$D_{\max}^2 = 1 - \frac{3}{2}p + \frac{3}{2}p^2, \quad B_{\max} = 2\sqrt{1 - 3p + 3p^2}. \quad (15)$$

*Example IV: Werner state.*—As a final example we consider the Werner state [40], which is defined as

$$\hat{\rho}_W(p) = \frac{1}{4}\begin{pmatrix} 1+p & 0 & 0 & 2p \\ 0 & 1-p & 0 & 0 \\ 0 & 0 & 1-p & 0 \\ 2p & 0 & 0 & 1+p \end{pmatrix} \text{ where } p \in \langle 0, 1\rangle.$$

$$(16)$$

The purity is $P = (1 + 3p^2)/4$. When this state is transformed, $D^2$ and $B_{\max}$ can attain any value inside the grey areas in Figs. 2(c) and 2(d). For these plots, the limits are

$$D_1 = D_2 = 0, \quad B_{\max} = 2\sqrt{2}p \quad (17)$$

for minimal coherence and maximal violation of the CHSH inequality and

$$D_{\max}^2 = p^2, \quad B_{\max} = 2p, \quad (18)$$

for maximal coherence and minimal violation of the CHSH inequality

*The relationship between coherence and correlations.*—For a given quantum state, the relationship between the degree of coherence of each subsystem and the correlations between subsystems is quantified by the measure $S_{A,B} = D_{A,B}^2/2 + \left(B_{\max}/2\sqrt{2}\right)^2$ called *accessible coherence* in the subsystem $A$, $B$ [24]. Especially, for a pure state the statement

$$\frac{D_{A,B}^2}{2} + \left(\frac{B_{\max}}{2\sqrt{2}}\right)^2 = 1 \quad (19)$$

is valid. Any increase (or decrease) of the degree of coherence is compensated by a corresponding change of $B_{\max}$. This relationship is no longer true for mixed states as shown in the Supplemental Material.

What is then, for all states, the appropriate equation that relates first-order coherence and correlations? For a generally mixed state ($\mathrm{Tr}\hat{\rho}^2 \leq 1$), one can derive [18]

$$\frac{D_A^2 + D_B^2}{4} + \mathcal{T} = \mathrm{Tr}\hat{\rho}^2, \quad (20)$$

where $\mathcal{T} = 1/4\left(1 + \sum_{i,j=1}^3 t_{ij}^2\right)$, $t_{ij} = \mathrm{Tr}\left[\hat{\rho}\hat{\sigma}_i \otimes \hat{\sigma}_j\right]$, and $\sigma_{i,j}$ ($i,j = 1, 2, 3$) are Pauli matrices. The values of $t_{ij}$ can only be obtained by making coincidence measurements between the subsystems, therefore measuring the nature of its correlations. In general

$$\frac{(\lambda_1 + \lambda_4)^2 + (\lambda_2 + \lambda_3)^2}{2} \leq \mathcal{T} \leq \mathrm{Tr}\hat{\rho}^2. \quad (21)$$

For a pure state, $D_A = D_B$ and $\mathcal{T} = (B_{\max}/2\sqrt{2})^2$, so one obtains Eq. (19). For maximally entangled states, $B_{\max} = 2\sqrt{2}$, so $\mathcal{T} = 1$ achieves its maximum value, while for separable pure states, $B_{\max} = 2$ and $\mathcal{T} = 1/2$.

*Conclusions.*—We have solved several puzzles about the relationship between coherence and certain measures of correlations present between subsystems, as it is the case of the CHSH inequality. For the case of two correlated two-dimensional subsystems, we have obtained simple expressions that quantify the amount of first-order coherence that can be obtained in each subsystem (*hidden coherence*) by modifying correlations between the subsystems. We have shown that the relevant parameter to quantify the maximum hidden coherence is the degree of violation of the CHSH inequality, not the degree of entanglement between subsystems. Although we have considered here only a few systems as examples, their analysis, based on suitably defined quantities, illuminates the general concept of extracting coherence from manipulating the correlations between subsystems.

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[39] In [24], $B_{\max}$ is calculated considering only projections into a subset (equivalent to considering only linear polarization states) of all the possible states that should be considered. However, the correct calculation of $B_{\max}$ needs to consider all possible measurements (projections), as shown in [18].

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# Revealing Hidden Coherence in Partially Coherent Light
## Supplemental Material

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Let $\hat{\rho}$ be a general 4 dimensional complex Hermitian matrix, that could represent a $2 \times 2$-dimensional mixed quantum state, or a partially coherent beam describing coherent or incoherent superpositions of four modes. In general, $\hat{\rho}$ can be always written as (*spectral decomposition*)

$$\hat{\rho} = V \hat{E} V^\dagger = \lambda_1 |a\rangle\langle a| + \lambda_2 |b\rangle\langle b| + \lambda_3 |c\rangle\langle c| + \lambda_4 |d\rangle\langle d|, \quad (1)$$

where the diagonal matrix $\hat{E}$ contains eigenvalues $\lambda_i$ and the matrix V consists of the corresponding eigenvectors $\{|a\rangle, |b\rangle, |c\rangle, |d\rangle\}$ forming an orthonormal basis. We assume that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ and $\sum_i \lambda_i = 1$. When a unitary transformation U is applied to the state $\hat{\rho}$, a new state $\hat{\rho}' = U \hat{\rho} U^\dagger$ is obtained,

$$\hat{\rho}' = \lambda_1 |a'\rangle\langle a'| + \lambda_2 |b'\rangle\langle b'| + \lambda_3 |c'\rangle\langle c'| + \lambda_4 |d'\rangle\langle d'|. \quad (2)$$

Notice that all states connected by the means of unitary transformations share the same eigenvalues, i.e., the eigenvalues $\lambda_i$ are invariant under the unitary transformations. However, the eigenvectors change.

## MINIMAL FIRST-ORDER COHERENCE

**Theorem:**

There exists a unitary transformation $U$ that when applied to $\hat{\rho}$ generates a new state $\hat{\rho}' = U \hat{\rho} U^\dagger$ so that the coherence $D$ vanishes and the violation of the CHSH is maximized with value [1, 2]

$$B_{\max} = 2\sqrt{2}\sqrt{(\lambda_1 - \lambda_4)^2 + (\lambda_2 - \lambda_3)^2}. \quad (3)$$

The unitary transformation has the form $U = MV^\dagger$, where

$$M = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & -1 & 0 & 0 \end{pmatrix}. \quad (4)$$

**Proof:**

First, we need to transform $\hat{\rho}$ to a diagonal form in the computational basis $\{|0\rangle_A|0\rangle_B, |0\rangle_A|1\rangle_B, |1\rangle_A|0\rangle_B, |1\rangle_A|1\rangle_B\}$. This is done with the help of the matrix $V$ that contains the eigenvectors of $\hat{\rho}$, so that

$$\hat{\rho} \to \hat{E} = V^\dagger \hat{\rho} V. \quad (5)$$

From [1], it can be shown that the violation of the CHSH inequality is maximized for a Bell diagonal state of the form

$$\hat{\rho} = \lambda_1 |\Phi^+\rangle\langle\Phi^+| + \lambda_2 |\Phi^-\rangle\langle\Phi^-|$$
$$+ \lambda_3 |\Psi^+\rangle\langle\Psi^+| + \lambda_4 |\Psi^-\rangle\langle\Psi^-|, \quad (6)$$

where $|\Phi^\pm\rangle$ and $|\Psi^\pm\rangle$ are the maximally entangled Bell states. Any unitary transformation applied on the state given by Eq. (6) cannot increase the degree of violation of the inequality.

A general Bell diagonal state in the computational basis writes as

$$\hat{\rho}_{\text{Bell}} = \frac{1}{2} \begin{pmatrix} \lambda_1 + \lambda_2 & 0 & 0 & \lambda_1 - \lambda_2 \\ 0 & \lambda_3 + \lambda_4 & \lambda_3 - \lambda_4 & 0 \\ 0 & \lambda_3 - \lambda_4 & \lambda_3 + \lambda_4 & 0 \\ \lambda_1 - \lambda_2 & 0 & 0 & \lambda_1 + \lambda_2 \end{pmatrix}. \quad (7)$$

The matrix $M$ performs the transformation [3]

$$\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} \Longrightarrow \{|\Phi^+\rangle, |\Phi^-\rangle, |\Psi^+\rangle, |\Psi^-\rangle\} \quad (8)$$

that can be easily demonstrated by direct inspection. After combining both transformations, now we have

$$\hat{\rho} \Longrightarrow \hat{\rho}' = M \hat{E} M^\dagger = M V^\dagger \hat{\rho} V M^\dagger. \quad (9)$$

The unitary transformation $U = MV^\dagger$ generates the state given in Eq. (6). From here, one can use the Horodecki's approach [2] to get Eq. (3) [1].

The coherence ($D$) for the state of the form given in Eq. (7) is

$$D_A^2 = 2\text{Tr}\left[\frac{1}{4}\begin{pmatrix} \sum_{i=1}^4 \lambda_i & 0 \\ 0 & \sum_{i=1}^4 \lambda_i \end{pmatrix}^2\right] - 1 = 0. \quad (10)$$

Similarly, we obtain $D_B^2 = 0$. That leads to $D^2 = (D_A^2 + D_B^2)/2 = 0$.

By means of a unitary transformation, we can generate a new state where both subsystems show no coherence $D = 0$. It corresponds to the state that shows the maximal violation of the CHSH inequality achievable for states connected through the unitary transformations.

## MAXIMAL FIRST-ORDER COHERENCE

**Theorem:**

There exists a unitary transformation $U$ that when applied to an arbitrary state $\hat{\rho}$ generates a new state $\hat{\rho}' = U\hat{\rho}U^{\dagger}$ that maximizes the coherence $D$ with value

$$D_{\max}^2 = (\lambda_1 - \lambda_4)^2 + (\lambda_2 - \lambda_3)^2 \qquad (11)$$

and yields a violation of CHSH that is minimal, with value

$$B_{\max} = 2\,|\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4|. \qquad (12)$$

The unitary transformation $U$ has the form $U = V^{\dagger}$.

**Proof:**

The unitary transformation $U = V^{\dagger}$ transforms an arbitrary state $\hat{\rho}$ into the state $\hat{E}$ that is diagonal in the computational basis $\{|0\rangle_A|0\rangle_B, |0\rangle_A|1\rangle_B, |1\rangle_A|0\rangle_B, |1\rangle_A|1\rangle_B, \}$, so it performs the transformation

$$\{|a\rangle, |b\rangle, |c\rangle, |d\rangle\} \implies \{|0\rangle_A|0\rangle_B, |0\rangle_A|1\rangle_B, |1\rangle_A|0\rangle_B, |1\rangle_A|1\rangle_B\}. \qquad (13)$$

Therefore

$$\hat{\rho} \implies \hat{\rho}' = V^{\dagger}\hat{\rho}V. \qquad (14)$$

One can see by performing extensive numerical simulations that the degree of coherence $D$ cannot be increased by applying additional unitary transformations $W$ on $\hat{E}$.

Moreover, when considering the Jarlskog recursive parametrization [4] of an arbitrary unitary transformation $W(\vec{\alpha})$ with parameter $\vec{\alpha}$, we can demonstrate that the function that gives the degree of coherence after the unitary transformation, $D[W(\vec{\alpha})\hat{E}W^{\dagger}(\vec{\alpha})]$ has a maximum for $\vec{\alpha} = 0$, which corresponds to the identity transformation, since

$$\left.\frac{\partial D\left[W(\vec{\alpha})\hat{E}W^{\dagger}(\vec{\alpha})\right]}{\partial\vec{\alpha}}\right|_{\vec{\alpha}=\vec{0}} = 0. \qquad (15)$$

Direct calculation of the Hessian matrix of second derivatives confirms that the state $\hat{E}$ has the maximal degree of coherence $D$. In this proof, alternating signs of the determinants of leading sub-matrices with the increasing rank have been obtained.

The degree of coherence $D$ of the state $\hat{E}$ with diagonal elements $\lambda_i$ is easily obtained to be

$$D_{\max}^2 = \frac{D_A^2 + D_B^2}{2} = (\lambda_1 - \lambda_4)^2 + (\lambda_2 - \lambda_3)^2. \qquad (16)$$

For the state $\hat{E}$, the only non-vanishing element of the matrix $T_{\rho}$ is $t_{33}$, that reads

$$T_{\hat{E}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \lambda_1 - \lambda_2 - \lambda_3 + \lambda_4 \end{pmatrix}. \qquad (17)$$
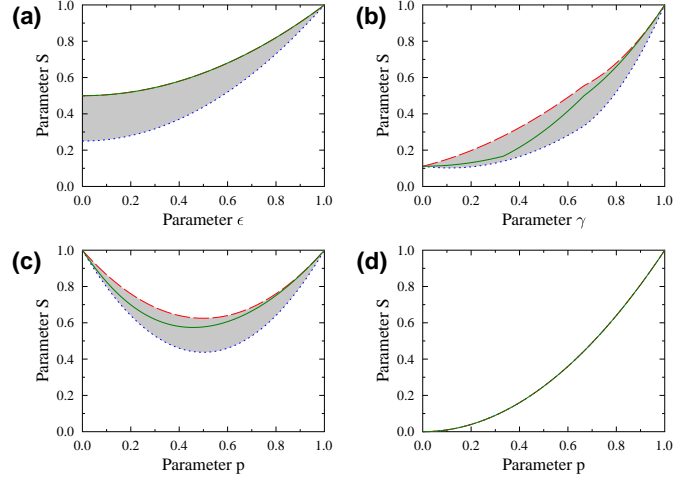


FIG. 1. Maximum and minimum values of $S$ for examples I-IV. (a) MNMS state, (b) MEMS state, (c) example C in [7] and (d) Werner state. The green line depicts the original value, prior to any unitary transformation. The dashed-red line depicts $S_{\max}$, and the dotted-blued line depicts $S_{\min}$. Grey areas mark all possible values of $S$.

The value of $B_{\max}$ is $B_{\max} = 2\sqrt{\mu}$, where $\mu = (\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4)^2$ is the only non-zero eigenvalue of $T_{\hat{E}}^T T_{\hat{E}}$. In this case

$$B_{\max} = 2|\lambda_1 - \lambda_2 - \lambda_3 + \lambda_4|. \qquad (18)$$

## GENERAL INVARIANT INVOLVING COHERENCE

One can be tempted to look for an expression similar to the one defined in [7] and define a parameter $S$ as

$$S = \frac{D_A^2 + D_B^2}{4} + \left(\frac{B_{\max}}{2\sqrt{2}}\right)^2. \qquad (19)$$

For certain states, it can be found that this parameter is indeed constant under unitary transformations. This is the case of the Werner state (example IV in the main text), as it is demonstrated below and can be observed in Fig. 1(d). However, in general, this is not the case. Examples I-III of the main text correspond to this situation, as it can be seen in Figs. 1(a)-(c), that show all possible values of $S$ (grey areas) obtained by unitary transformations.

It can be easily shown using Eqs.(1)-(4) of the main text that all values of $S$ are between upper and lower boundaries: $S_{\max} = P - 2(\lambda_1\lambda_4 + \lambda_2\lambda_3)$ and $S_{\min} = P - (\lambda_1 + \lambda_4)(\lambda_2 + \lambda_3)$, where $P$ stands for the purity of the state. $S_{\max}$ corresponds to the maximal violation of the CHSH inequality and the minimal first-order coherence,

whereas $S_{\min}$ corresponds to the minimal violation of the CHSH inequality and the maximal first-order coherence.

For a general mixed state ($\mathrm{Tr}\hat{\rho}^2 \leq 1$), one can derive [2]

$$\frac{D_A^2 + D_B^2}{4} + \mathcal{T} = \mathrm{Tr}\hat{\rho}^2, \tag{20}$$

where $\mathcal{T} = 1/4\left(1 + \sum_{i,j=1}^{3} t_{ij}^2\right)$, $t_{ij} = \mathrm{Tr}\left[\hat{\rho}\hat{\sigma}_i \otimes \hat{\sigma}_j\right]$ and $\sigma_{i,j}$ $(i,j = 1,2,3)$ are the Pauli matrices. The values of $t_{ij}$ can be only obtained by making coincidence measurements between the subsystems, therefore measuring the nature of their correlations. Any increase/decrease of the degree of coherence is accompanied by a corresponding decrease/increase of $\mathcal{T}$. For a pure state, $D_A = D_B$ and $\mathcal{T} = (B_{\max}/2\sqrt{2})^2$ (see below), so one obtains

$$\frac{D_{A,B}^2}{2} + \left(\frac{B_{\max}}{2\sqrt{2}}\right)^2 = 1. \tag{21}$$

### PURE STATES: DERIVATION OF EQ. (21)

Any pure state can be written as a Schmidt decomposition that reads [5]

$$|\Psi\rangle = \kappa_1 |x_1\rangle_A |y_1\rangle_B + \kappa_2 |x_2\rangle_A |y_2\rangle_B, \tag{22}$$

where $\kappa_1^2 + \kappa_2^2 = 1$, $\{|x_1\rangle_A, |x_2\rangle_A\}$ is an orthonormal basis in subsystem $A$ and $\{|y_1\rangle_B, |y_2\rangle_B\}$ is an orthonormal basis in subsystem $B$. For the sake of simplicity we assume $\kappa_{1,2}$ to be real. Following [6], one obtains that

$$\sum_{i,j=1}^{3} t_{ij}^2 = 1 + 8\kappa_1^2\kappa_2^2, \tag{23}$$

$$B_{\max} = 2\sqrt{1 + 4\kappa_1^2\kappa_2^2}. \tag{24}$$

Therefore

$$\mathcal{T} = \frac{1 + \sum_{i,j=1}^{3} t_{ij}^2}{4} = \frac{1 + 4\kappa_1^2\kappa_2^2}{2}$$
$$= \frac{1}{2}\left[1 + \left(\frac{B_{\max}^2}{4} - 1\right)\right] = \left(\frac{B_{\max}}{2\sqrt{2}}\right)^2 \tag{25}$$

Substitution of Eq. (25) into Eq. (20) yields straightforwardly Eq. (21).

### WERNER STATE: INVARIANCE OF THE PARAMETER $S$ UNDER GLOBAL UNITARY TRANSFORMATIONS

The Werner state (example IV of the main paper) can be written as [8]

$$\hat{\rho}_W = \frac{1-p}{4}I_4 + p|\Phi^+\rangle\langle\Phi^+|, \tag{26}$$

where $|\Phi^+\rangle = 1/\sqrt{2}\left(|0\rangle_A|0\rangle_B + |1\rangle_A|1\rangle_B\right)$ is the maximally entangled Bell state. The Werner state can be generalized considering the state $|\Psi\rangle$ given by Eq. (22) instead of $|\Phi^+\rangle$. The spectral decomposition of the generalized state can be written as

$$\hat{\rho}_W = \frac{1+3p}{4}|\Psi\rangle\langle\Psi| + \frac{1-p}{4}|\Psi^\perp\rangle\langle\Psi^\perp| \tag{27}$$
$$+ \frac{1-p}{4}\left(|x_1\rangle_A|y_2\rangle_B\langle x_1|_A\langle y_2|_B + |x_2\rangle_A|y_1\rangle_B\langle x_2|_A\langle y_1|_B\right),$$

where $|\Psi^\perp\rangle = -\kappa_2|x_1\rangle_A|y_1\rangle_B + \kappa_1|x_2\rangle_A|y_2\rangle_B$. The corresponding matrix $T_\rho$ writes

$$T_\rho = \begin{pmatrix} 2p\kappa_1\kappa_2 & 0 & 0 \\ 0 & -2p\kappa_1\kappa_2 & 0 \\ 0 & 0 & p \end{pmatrix}. \tag{28}$$

The maximal violation of the CHSH inequality writes

$$B_{\max} = 2p\sqrt{1 + 4\kappa_1^2\kappa_2^2} \tag{29}$$

and

$$\mathcal{T} = \frac{1 + p^2 + 8p^2\kappa_1^2\kappa_2^2}{4}. \tag{30}$$

Substituting Eq. (30) into Eq. (20), and making use of Eq. (29), one obtains that

$$\frac{D^2}{2} + \left(\frac{B_{\max}}{2\sqrt{2}}\right)^2 = p^2. \tag{31}$$

For $p = 1$ (pure state) we recover Eq. (21).

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